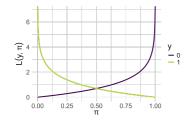
Introduction to Machine Learning

Advanced Risk Minimization Proper Scoring Rules





Learning goals

- Honest probabilistic forecasts
- Proper scoring rules
- log score
- Brier score

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Scoring rules S(P,y) assess the quality of probabilistic forecasts by assigning a score based on the predictive distribution P and the realized event y. The expected score w.r.t. the RV $y \sim Q$ is denoted as

$$S(P,Q) = \mathbb{E}_{y \sim Q}[S(P,y)]$$

A scoring rule is **proper** if the forecaster maximizes the expected score for an observation drawn from Q if he or she issues the forecast Q rather than $P \neq Q$:

$$S(Q,Q) \geq S(P,Q)$$
 for all P,Q

S is **strictly proper** when equality holds iff P = Q. (Strictly) proper scores ensure the forecaster has an incentive to predict Q and is encouraged to report his or her true belief.

NB: scores are typically positively oriented (maximization) while losses are negatively oriented (minimization). Scores could also be defined negatively oriented.



For simplicity, we will only look at binary targets $y \sim \text{Bern}(p)$. We want to find out if using a loss $L(y,\pi)$ (negative score) incentivizes honest forecasts $\pi = p$ for any $p \in [0,1]$.



For any loss *L*, its expectation w.r.t. *y* is

$$\mathbb{E}_{y}[L(y,\pi)] = p \cdot L(1,\pi) + (1-p) \cdot L(0,\pi)$$

Let's first look at a negative example. Assuming the **L1 loss** $L(y,\pi)=|y-\pi|$, we obtain

$$\mathbb{E}_{y}[L(y,\pi)] = \rho|1-\pi| + (1-\rho)\pi = \rho + \pi(1-2\rho)$$

The expected loss is linear in π , hence we minimize it by setting $\pi=1$ for p>0.5 and $\pi=0$ for p<0.5.

The score $S(\pi, y) = -L(y, \pi)$ is therefore not proper.

The **0/1 loss** $L(y,\pi) = \mathbb{1}_{\{y \neq h_{\pi}\}}$ using the discrete classifier $h_{\pi} = \mathbb{1}_{\{\pi > 0.5\}}$ yields in expectation over y:

$$\mathbb{E}_y[L(y,\pi)] = p \cdot L(1,\pi) + (1-p) \cdot L(0,\pi)$$

$$= \begin{cases} p & \text{if } h_\pi = 0 \\ 1-p & \text{if } h_\pi = 1 \end{cases}$$

- For p > 0.5 we minimize the expected loss by choosing $h_{\pi} = 1$, which holds true for any $\pi \in (0.5, 1)$
- Likewise for $p \le 0.5$, any $\pi \in (0, 0.5]$ minimizes the expected loss

The **0/1 score** (negative 0/1 loss) is therefore proper but not strictly proper since there is no unique maximum.



To find strictly proper scores/losses, we can ask: Which functions have the property such that $\mathbb{E}_y[L(y,\pi)]$ is minimized at $\pi=p$? We have

$$\mathbb{E}_{y}[L(y,\pi)] = p \cdot L(1,\pi) + (1-p) \cdot L(0,\pi)$$

Let's further assume that $L(1,\pi)$ and $L(0,\pi)$ can not be arbitrary, but are the same function evaluated at π and $1-\pi$: $L(1,\pi)=L(\pi)$ and $L(0,\pi)=L(1-\pi)$. Then

$$\mathbb{E}_{y}[L(y,\pi)] = p \cdot L(\pi) + (1-p) \cdot L(1-\pi)$$

Setting the derivative w.r.t. π to 0 and requiring $\pi = p$ at the optimum (**propriety**), we get the following first-order condition (F.O.C.):

$$p \cdot L'(p) \stackrel{!}{=} (1-p) \cdot L'(1-p)$$



- F.O.C.: $p \cdot L'(p) \stackrel{!}{=} (1-p) \cdot L'(1-p)$
- One natural solution is L'(p) = -1/p, resulting in -p/p = -(1-p)/(1-p) = -1 and the antiderivative $L(p) = -\log(p)$.



• This is the log loss

$$L(y,\pi) = -(y \cdot \log(\pi) + (1-y) \cdot \log(1-\pi))$$

 The corresponding scoring rule (maximization) is the strictly proper logarithmic scoring rule

$$S(\pi, y) = y \cdot \log(\pi) + (1 - y) \cdot \log(1 - \pi)$$

- F.O.C.: $p \cdot L'(p) \stackrel{!}{=} (1-p) \cdot L'(1-p)$
- A second solution is L'(p) = -2(1-p), resulting in -2p(1-p) = -2(1-p)p and the antiderivative $L(p) = (1-p)^2 = \frac{1}{2}((1-p)^2 + (0-(1-p))^2)$



 This is also called the Brier score and is effectively the MSE loss for probabilities

$$L(y,\pi) = \frac{1}{2} \sum_{i=1}^{2} (y_i - \pi_i)^2$$

(with
$$y_1 = y, y_2 = 1 - y$$
 and likewise $\pi_1 = \pi, \pi_2 = 1 - \pi$)

• Using positive orientation (maximization), this gives rise to the **quadratic scoring rule**, which for two classes is $S(\pi, y) = -\frac{1}{2} \sum_{i=1}^{2} (y_i - \pi_i)^2$